Informatics V - Chair of Scientific Computing
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Coupled Approaches for Fluid Dynamic Problems Using the PDE Framework Peano

The Peano Framework

- Framework for multiscale, parallel PDE solvers using dynamically adaptive Cartesian grids [8]
- Support of arbitrary dimensional grids
- Low memory footprint
- Grid traversal along Peano curve yields high cache efficiency
- Encapsulation of PDE solvers in different components
- Various solvers/applications:
  - Multigrid Poisson solver [8]
  - Finite Element solver for the Navier-Stokes equations [5]
  - Lattice Boltzmann automaton
  - Spatiotemporal multigrid solver for the heat equation

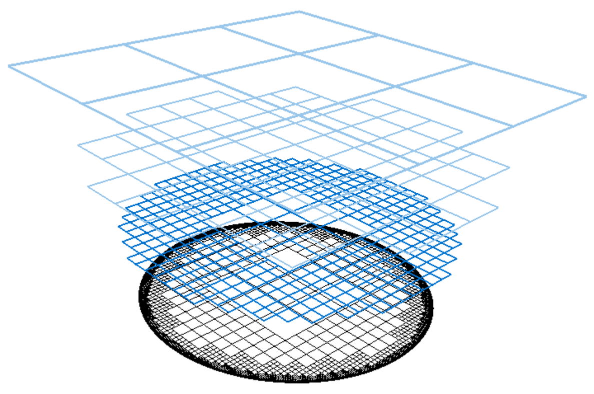


Figure 1: Multiscale representation of the circular domain [8]

The Lattice Boltzmann Method

$$
\begin{aligned}
f_i(x+c_i\cdot dt, t+dt) &= f_i^{eq}(x,t) + \Delta_i(f(x,t) - f^{eq}(x,t)) \\
&\Updownarrow \\
f_i^*(x,t) &= f_i^{eq}(x,t) + \Delta_i(f(x,t) - f^{eq}(x,t)) \quad \text{Collide step} \\
f_i(x+c_i\cdot dt, t+dt) &= f_i^*(x,t) \quad \text{Streaming step}
\end{aligned}
$$

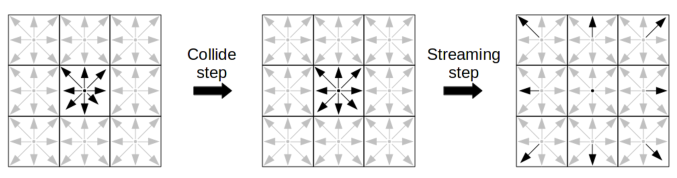
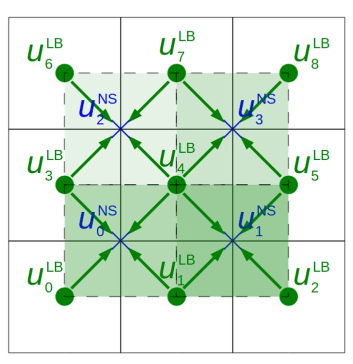


Figure 2: Pre-Collision (left), Post-Collision (center) and Post-Streaming state (right) in the LB-algorithm

- Compute probability $f_i(x,t)$ for finding fluid molecules with velocity c_i in small surrounding of x at time t $(i = 1, ..., Q)$
- Modeling of intermolecular collisions by linear collision operator $\Delta(f - f^{eq})$
- Convective transport by streaming f_i to neighbouring cells

Coupling: Lattice Boltzmann → Navier-Stokes



- Reconstruct velocities u^{NS} from u^{LB}:
  - Rescale lattice velocity values $u^{LB} := u_L^{LB} \cdot \frac{dx}{dt}$
  - Compute u^{NS} from bilinear interpolation applied to LB velocity values u^{LB}
- No pressure coupling $p^{LB} \to p^{NS}$ required

Figure 3: Coupling of the velocities $u^{LB} \to u^{NS}$

Coupling: Navier-Stokes → Lattice Boltzmann

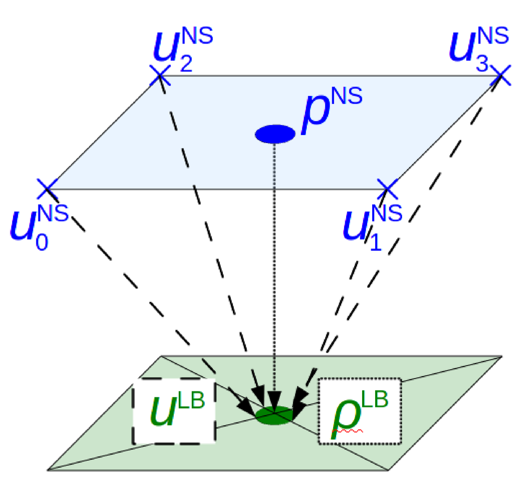


Figure 4: Mapping of p^{NS}, u^{NS} onto ρ^{LB}, u^{LB}

- Split $f_i = f_i^{eq}(\rho^{LB}, u^{LB}) + f_i^{neq}$
- Determine ρ^{LB}, u^{LB} from p^{NS}, u^{NS}
- Solve minimisation problem

$$\min_{f^{neq}\in\mathbb{R}^Q} g(f^{neq}) \quad \text{such that}$$

$$
\begin{aligned}
\sum_i f_i^{neq} &= 0 \\
\sum_i f_i^{neq} c_{i_\alpha} &= 0 \\
-\frac{1}{2}\sum_i \left(2f_i^{neq} + \Delta_i(f^{neq})\right) c_{i_\alpha} c_{i_\beta} &= \nu\left(\frac{\partial u_\beta^{NS}}{\partial x_\alpha} + \frac{\partial u_\alpha^{NS}}{\partial x_\beta}\right), \\
&\alpha, \beta \in \{1, ..., d\}
\end{aligned}
$$

- $g(f^{neq}) \in \{h : \mathbb{R}^Q \to \mathbb{R},\ h(f^{neq}) = \sum_{i\le j} d_{ij} f_i^{neq} f_j^{neq} + \sum_i d_i f_i^{neq} + d_0$ with $d_{ii} > 0\ \forall i\}$
- Choice for g: $g(f^{neq}) = \sum_i \left(\frac{f_i^{neq}}{f_i^{eq}}\right)^2$

Motivation

Many flow systems – especially in micro- and nano-fluidics – are strongly influenced by physical processes that appear on different spatial and temporal scales. Flows through nanopores or in porous media influenced by Brownian motion effects are typical examples. Solving these kinds of complex systems by means of computational fluid dynamics (CFD) often requires highly adaptive concepts or different sorts of solvers depending on the current scale to be simulated.

In this contribution, we couple different flow models using the PDE framework Peano [8] as a common base. Based on an octree-like adaptive grid generation approach, Peano allows for multiscale simulations and massively parallel computations. Moreover, it comprises several PDE solvers encapsulated in single components, amongst others a CFD component based on a Navier-Stokes (NS) finite element method [5] and a component for solving mesoscopic flow problems by the Lattice Boltzmann method (LB). The present contribution describes the Lattice Boltzmann component and the LB-NS-coupling approach combining the LB and the NS component.

Lattice Boltzmann Simulations in Peano: Features

- Adaptive LB simulations based on a volumetric approach [6]
- Encapsulation of collision models and boundary conditions in separate management systems
  → Easy exchange/ removal/ extension of the current models/ boundary conditions
- Available collision models:
  - BGK collision model [2]
  - Multiple-relaxation-time model proposed by d'Humières et al. [4]
  - Fluctuating model capturing Brownian motion effects in the fluid [3]
- Support of arbitrary direct-neighbour velocity discretisation schemes in 2D/3D (D2D9, D3Q15,D3Q19,D3Q27,...)
- AA-storage pattern for particle distribution functions yields low memory footprint [1]
- Coupling to NS-solver
- Free surface extension [7] for regular Cartesian grid
- VTK-compatible multilevel-output for postprocessing

Results: Solver Coupling

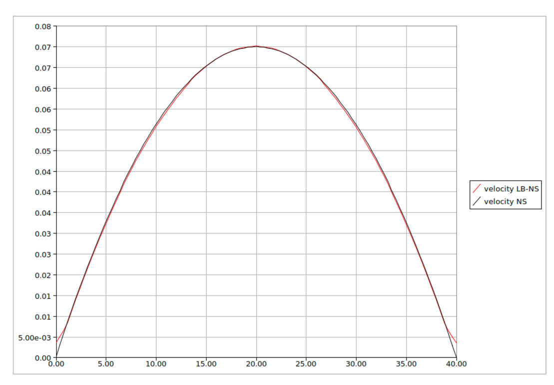


Figure 5: Velocity profile of NS and LB-NS simulations in a 2D channel flow.

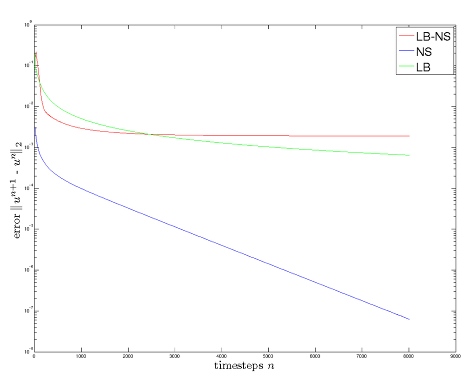


Figure 6: Error in velocity profile in NS, LB and LB-NS simulations

Outlook: Adaptive Multiscale Simulations

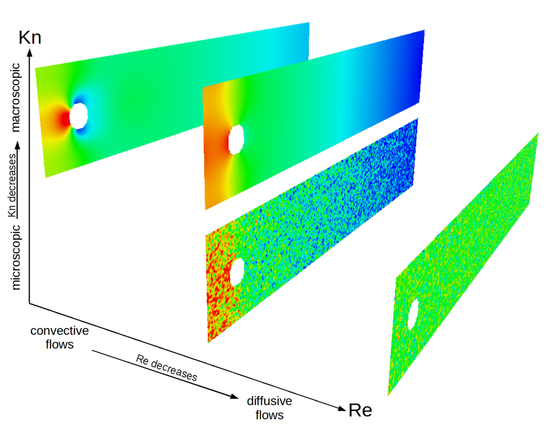


Figure 7: Channel flow simulations on different scales. For higher Knudsen numbers, Brownian effects are taken into account.

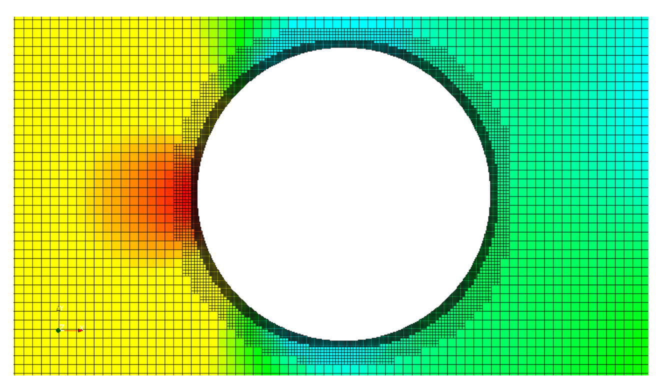


Figure 8: Density distribution at a spherical obstacle in a Karman vortex flow simulation at Re=100 on a three-level grid

References

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